Upgrading of a Neutron Diffractometer at Los Alamos Neutron Science Center for Materials Research and Education

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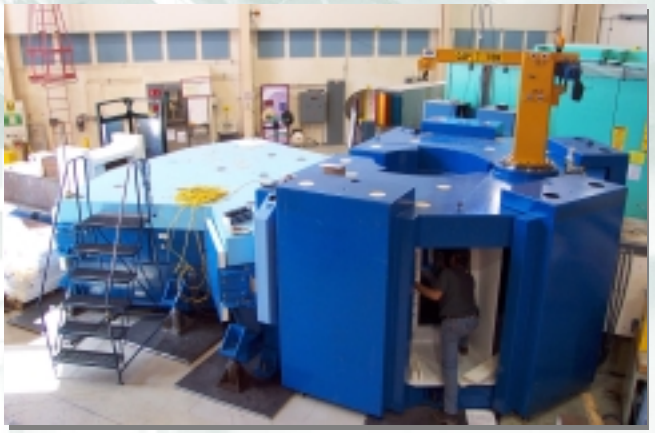
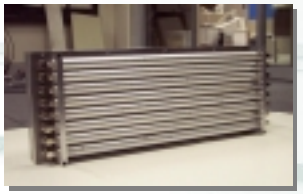
Recent Activities

Knowing the atomic structure of materials usually means determining the crystal structure. However, many modern materials are complex, and their real structure often is deviated locally from the average crystal structure in significant ways. It is thus necessary to know the structure on **various length scales,** including **local atomic arrangements** that more directly govern properties**.** But the conventional crystallographic approach cannot provide a complete picture; it has to be complemented by local probes such as the **Pair Distribution Function (PDF) method**. We are currently upgrading the instrument NPD at the Lujan Canter of Los Alamos National Lab. to become **NPDF**, an instrument dedicated to the high-resolution PDF method. This upgrade will not only put NPDF at the cutting edge of local structure determination but also serve as development platform for this new structure analysis tool for **nano-structured materials**.





***Above*: The NPDF Instrument at Lujan Center, Los Alamos National Lab.**
***Left*: Detector panel holding eight position sensitive ^{3}He detectors.**

SRO ⟵ Nano-Scale Atomic Structure

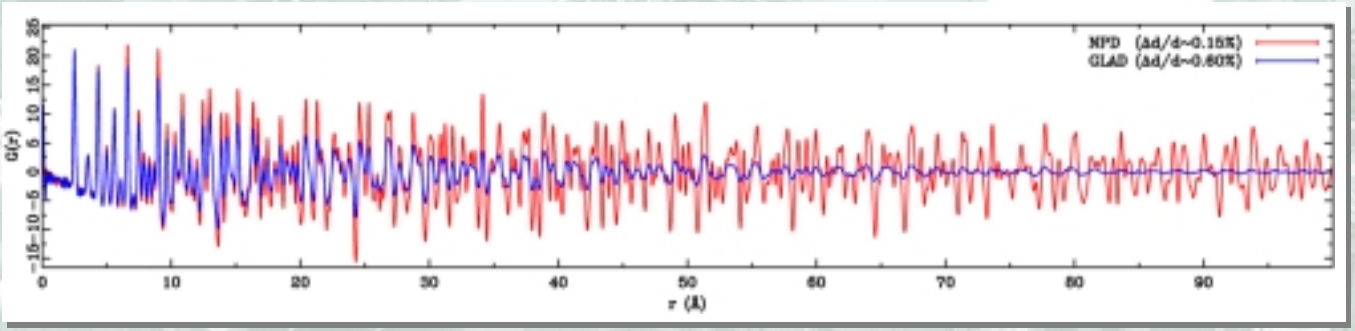


Figure on the left compares PDFs for Nickel from high-resolution NPD and low-resolution GLAD. The data from NPD give information on short range order (SRO) as well as nano-scale atomic structure.

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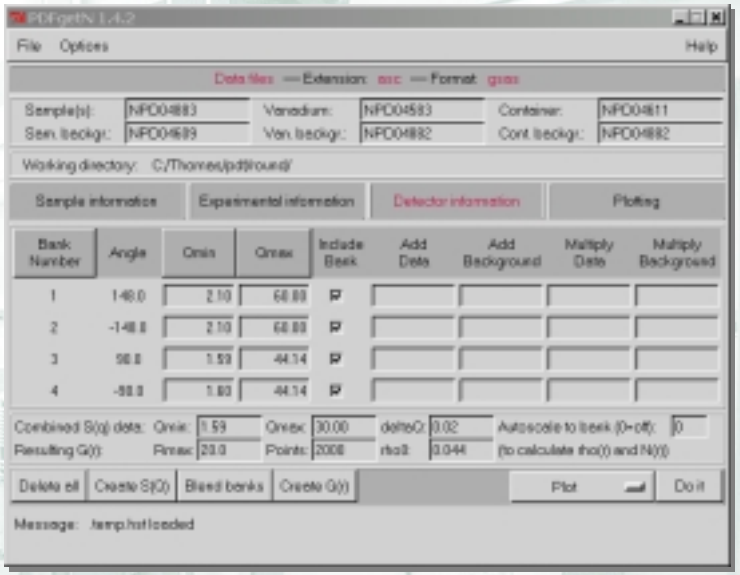
Education, Outreach and Mentoring

The current curriculum in physics, material science or chemistry focuses on the traditional crystallographic approach to structure determination. With modern materials getting more **disordered** or in the case of **nano-crystals** being **"crystallographycally challenged"** crystals all together, there is a growing need to educate young scientists in total scattering techniques such as the PDF method. In July 2001 a very successful one-day workshop about the PDF method was held as part of the Annual Crystallographic Meeting in Los Angeles.

***Top*: Cover of PDF workshop CDROM. *Left*: Simon Billinge (right) and some participants.**



A vital part in the success of the PDF method and the upgraded NPDF is **user-friendly** data processing and modeling software. The picture above show a screenshot of the PDF processing program **PDFgetN**.

P.F. Peterson, M. Gutmann, Th. Proffen and S.J.L. Billinge, *J. Appl. Cryst.* **33**, 1192 (2000).